REVIEW OF VARIOUS LATTICE DYNAMICAL MODELS

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Abstract

Alkali metals have played a significant role in the development of various lattice dynamical theories because of the simplicity of the electronic structure of their atoms and the high degree of symmetry associated with their atomic arrangement. The lattice dynamical study of metals has attracted the maximum theoretical attention in the past because of availability of experimental data along the principal symmetry directions using the inelastic scattering of neutrons by phonon for their comparison with theoretical results. The purpose of this paper is to study the lattice dynamics of metals with the help of force constant models viz. central force model, De Launay angular force model, CGW angular force model and Axial symmetric model etc. These models were proposed on the basis of different assumptions regarding the nature and range of their interactions. In the present study various lattice dynamical models have been reviewed. The ultimate aim of this research is to study various properties of metals on the basis of these proposed models.

Keywords: *Alkali Metals, Inelastic Scattering, Interactions, Lattice Dynamics, models*

1. Introduction

In the recent years, there has been an increasing demand for special materials for the development of highly sophisticated devices and gadgets. This has resulted in the emergence of new branch of science known as ***"Material Science".*** Material science seeks to understand what makes one material behave differently from another. Such understanding implies the prediction of the macroscopic behavior of matter in terms of fundamental microscopic concepts such as crystal structure and interatomic forces. This provides an efficient approach to this branch of science.

When several atoms bind together, a chunk of a solid material is formed where the atoms are held together by the delicate interplay of interatomic forces. But we know only this and nothing more. One of the ways to probe in to the nature of the interatomic forces is to disturb the equilibrium configuration of atoms in the solid and observe how the interatomic forces react to the disturbance. This leads us to the field of ***Lattice Dynamics***.

Many physical properties of solids are directly dependent upon their atomic arrangement and the corresponding crystal structure. In order to develop any new material with specific properties, it is essential to understand the relation between the macroscopic properties exhibited by a solid and the interatomic forces which holds its atoms together. However, the

nature of these forces has eluded exact description even in case of alkali metals. One of the ways to probe in to their nature and range is to disturb the equilibrium configuration of atoms in a solid and to study the oscillations set up by the unbalanced forces.

It is however, necessary to compare the theoretically deduced permissible frequencies of solids with the corresponding experimental data, to extract any information regarding the nature and range of interatomic forces. In the early days of lattice dynamics there was no experimental data either on the frequency spectra or the dispersion relations of solids. The sole aim of lattice dynamical theories in those days was to explain the observed variation of specific heat as a function of temperature. However, the specific heat being an average property is insensitive to the details of the frequency spectrum of a solid and nature of interatomic forces.

The measurement of phonon frequencies of most metals along the principal symmetry directions using the inelastic scattering of neutrons during the past few decades. That measurement has stimulated the interest in the lattice dynamical study of metals. The potential energy of a crystal consisting of N atoms is invariably a function of the position coordinates of its atoms. It can be expressed as a sum of two body, three body, four body and ultimately N- body interaction potential energies. All phenomenological theories assume that the potential energy of a crystal can be expressed in terms of two body interactions.

Besides, it is necessary to make certain assumptions regarding the nature of atomic interactions in order to express the potential energy in terms of force constants of a lattice dynamical model. Each of these models is based on a specific assumption regarding the nature of interatomic forces and the number of force constants in a model varies with the range of these forces. The validity of a force constant model is usually judged by comparing its dispersion curves with the experimental ones.

These models for metals split the total atomic interactions in to short range ion- ion interactions and the long range electron –ion interactions. The ion–ion interactions are expressed in terms of variety of two body forces while the electron-ion interactions are expressed in terms of volume forces.

2. Review of Previous Work Based on Force Constants Models

*2.*1. Central Force Model

This model is based upon the simplest assumption regarding the nature of interatomic forces. It depends on the distance between the atoms only, but not on its orientation in space. As consequences, only one force constant which is related to the second derivative of the potential energy is associated with each set of neighbors. Bauer was the first to use this model with the range of interaction extended up to second nearest neighbors in the lattice dynamical study of sodium. If the interactions between the atoms of a monatomic crystal are described by central forces, it can be deduced that certain relations must exist between the elastic constants. They are known as Cauchy relations, after their discoverer. For a cubic crystal, there is only one Cauchy relation, namely

$$C_{12} = C_{44}$$

But the earlier determined values of elastic constants are not generally satisfied with the above Cauchy relation. But it was found that for most of the metals $C_{12} > C_{44}$, whereas for diamond, Ge & Si we see that $C_{12} < C_{44}$. These equations are not consistent with Cauchy

Relation for cubic crystal. So the interaction between the atoms of the elements can't described by central forces. This is called as Cauchy discrepancy.

However, the observed Cauchy discrepancies of alkali metals were not consistent with this model. Other workers removed this difficulty by including the volume forces due to electrons, which cannot be expressed in terms of central forces. Nevertheless, this model was found to be inadequate to explain the phonon dispersion curves or the specific heat in the low temperature region of the alkali metals. Hence this crude and unrealistic model has not been used in the present study.

2.2. Delaunay Angular Force Model

In this model the atomic interactions are expressed in terms of central forces and angular forces. Delaunay treated the angular forces by considering the relative displacement of the bond line between two atoms with respect to its equilibrium position. The components of this relative displacement parallel and perpendicular to the equilibrium bond line give rise to central and angular forces respectively. Their description, therefore involves one central and one angular force constant for each set of neighbors, respectively.

The two angular force constants along two mutually perpendicular directions become equal in the case of cubic symmetry and as a consequence the total number of force constants is reduced. In the present work, this model has been used to calculate the phonon frequencies of Sodium by restricting the range of ion –ion interactions up to third nearest neighbors. The choice of Sodium for the present work is because Sodium is the best example of free electrons.

2.3 CGW Angular Force Model

The atomic interactions in this model are proposed by Clark etal in terms of central forces and angular forces respectively, along and perpendicular to the line joining the atoms. However, unlike the DAF models, Clark considered the angular forces which depend upon the changes in the angles of the triangle which obtained by joining the equilibrium positions of these atoms on the plane of their equilibrium positions. However, these central forces are in no way different from those in DAF model. But this model doesn't consider the angular forces perpendicular to the plane of the triangles. Hence their description involves one central force constant for each set of neighbors. On the other hand the number of angular force constants in this model depends upon the number of triangles considered.

A variety of triangles can be formed by bond lines between different kinds of neighbors. However, the number of force constants which can be evaluated using the available experimental data that determine the actual number of triangles included in the sum. Clark, who developed this angular force model, did not investigate the lattice dynamics of alkali metals using this model. However, this model has been used by others in the Lattice Dynamical study of Lithium, Sodium, Potassium and rubidium but not in case of Cesium.

2.4 Axially Symmetric Model

This model assume that the interatomic forces are symmetric about the equilibrium bond line between two atoms and therefore require two force constants for each set of neighbor to describe the atomic interactions along and perpendicular to the equilibrium bond line. On the basis of this model in which the range of interactions was confined to first two neighbors while the volume forces were included to take care of electron-ion interactions. The five force constants were evaluated using the three elastic constants and two zone boundary frequencies. The theoretical phonon frequencies of sodium and potassium were in very good agreement with their experimental values. Hence the atomic interactions are expressed in terms of axially symmetric forces. The description of atomic interactions involves bond bending and bond stretching forces. Bond bending forces associated with the displacements perpendicular to the equilibrium bond line and Bond stretching forces parallel to the equilibrium bond line.

2.5 Other Force Constant Models

In addition to these models described above, there are other force constant models with their own assumptions regarding the interatomic forces, which have been used in the lattice dynamical study of alkali metals. However, these models are not described here, mainly because they are either related to one of the models described earlier or not radically different from the later. In any case they do not provide us any new information regarding the nature of atomic interaction.

2.6 Pseudopotential Models

These models express the atomic interactions in terms of ion-ion core repulsion, ion-ion core coulomb interaction and ion-electron-ion interactions. This thesis doesn't describe any of these pseudopotential models or the procedure followed by them to deduce the phonon frequencies, mainly because the present investigations on lattice dynamics of alkali metals are based on phenomenological approach. Experimental data for the phonon frequencies of alkali metals was obtained using inelastic scattering of neutron by phonon.

3. Inelastic Scattering of Neutron by Phonon

It is the most common method for the experimental determination of phonon dispersion relation. But this method is not applicable when absorption of neutron takes place by the nuclei of the crystal is high. Let us consider a neutron interact with a crystal and is scattered in elastically. In this process neutron will loss or gain the energy and momentum. This loss or gain corresponds to creation or absorption of one phonon. The kinematics of the scattering of a neutron beam by a crystal lattice is described by the general wave vector.

$$\vec{K} + \vec{G} = \vec{K}' \pm \vec{R}$$

Where $\vec{K} \rightarrow$ Wave vector of incident neutron

$\vec{G} \rightarrow$ Reciprocal lattice vector

$\vec{K}' \rightarrow$ Wave vector of scattered neutron

$\vec{R} \rightarrow$ Wave vector of phonon

Positive and negative symbol correspond to a phonon created or absorbed respectively. The choice of $\vec{G}$ in such a way that $\vec{R}$ lies in first Brillouin zone. Absorption or emission can be done between nearest neighbors only.

Let M_n be the mass of neutron. Then kinetic energy of incident neutron is

$$\frac{P^2}{2M_n} = \frac{\hbar^2 K^2}{2M_n}$$

Momentum of incident neutron = $\hbar\vec{K}$

Kinetic energy of scattered neutron = $\frac{\hbar^2 K'^2}{2M_n}$

By applying law of conservation of energy:

$$\frac{\hbar^2 K'^2}{2M_n} \pm \hbar\omega = \frac{\hbar^2 K^2}{2M_n}$$

$\pm\hbar\omega \rightarrow$ Energy of phonon created or absorbed respectively.

4. Conclusions

This review reveals that Central force model is based upon the simplest assumption regarding the nature of interatomic forces. It depends on the distance between the atoms only, but not on its orientation in space. As a consequence, only one force constant which is related to the second derivative of the potential energy, is associated with each set of neighbors. In De Launay Angular Force model, the atomic interactions are expressed in terms of central forces and angular forces. Delaunay treated the angular forces by considering the relative displacement of the bond line between two atoms with respect to its equilibrium position. The components of this relative displacement parallel and perpendicular to the equilibrium bond line give rise to central and angular forces respectively. Their description, therefore involves one central and one angular force constant for each set of neighbors, respectively. In CGW Angular Force Model, the atomic interactions in this model are expressed in terms of central forces and angular forces acting, respectively, along and perpendicular to the line joining the atoms. However, unlike the De Launay Angular Force models, Clark etal considered the angular forces which depend upon the changes in the angles of the triangle which obtained by joining the equilibrium positions of these atoms on the plane of their equilibrium positions. However, these central forces are in no way different from those in DAF model. But these models don't consider the angular forces perpendicular to the plane of the triangles. In Axial

Symmetric model, it assumes that the interatomic forces are symmetric about the equilibrium bond line between two atoms and therefore require two force constants for each set of neighbor to describe the atomic interactions along and perpendicular to the equilibrium bond line. On the basis of model in which the range of interactions was confined to first two neighbors while the volume forces were included to take care of electron-ion interactions. The purpose of this review is to study the lattice dynamics of metals with the help of these above mentioned models.

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